

## Author Index to Volume 167

Aiga, F., K. Sasagane and R. Itoh, The quadratic response function in the TDHF approximation and its application to frequency-dependent hyperpolarizabilities of the FH molecule	167 (1992) 277
Allan, M., see O. Schafer	167 (1992) 241
Bacska, G.B., see J.S. Craw	167 (1992) 77
Bacska, G.B., see J.S. Craw	167 (1992) 101
Baklanov, A.V., see A.B. Vakhtin	167 (1992) 1
Balavoine, G., see R. Loucif-Saibi	167 (1992) 369
Ballard, C.C., see I.C. Walker	167 (1992) 61
Bandyopadhyay, T. and K.V.S. Rama Rao, Excitation transfer by long-range and short-range interactions in liquid solution: the temporal behavior	167 (1992) 131
Banerjee, A., see R.C. Boehm	167 (1992) 291
Boczar, M., see J. Najbar	167 (1992) 37
Boehm, R.C. and A. Banerjee, Ab initio study of the oxides of rhenium and their anions	167 (1992) 291
Bonazzola, L., see R. Loucif-Saibi	167 (1992) 369
Bonomo, R.P., A.J. Di Bilio and F. Riggi, EPR investigation of chromium (III) complexes: analysis of their frozen solution and magnetically dilute powder spectra, <i>Chem. Phys.</i> 151 (1991) 323. Erratum	167 (1992) 385
Boutalib, A., J.P. Daudey and M. El Mouhtadi, Theoretical study of the lowest electronic states of CaH and CaH <sup>+</sup> molecules	167 (1992) 111
Boyarskaya, I.A., see O. Schafer	167 (1992) 241
Brion, C.E., see G.R. Burton	167 (1992) 349
Burton, G.R., W.F. Chan, G. Cooper and C.E. Brion, Absolute oscillator strengths for photoabsorption (6–360 eV) and ionic photofragmentation (10–80 eV) of methanol	167 (1992) 349
Cerny, T.M., see T.-Y.D. Lin	167 (1992) 203
Chan, W.F., see G.R. Burton	167 (1992) 349
Cooper, G., see G.R. Burton	167 (1992) 349
Cormican, H.F.J., see I.T.F. Gillan	167 (1992) 193
Coxon, J.A. and P.G. Hajigeorgiou, On the direct determination of analytical diatomic potential energy functions from spectroscopic data: the X <sup>1</sup> Σ <sup>+</sup> electronic states of NaF, LiI, CS, and SiS	167 (1992) 327
Craig, D.P. and T. Thirunamachandran, An analysis of models for resonant transfer of excitation using quantum electrodynamics	167 (1992) 229
Craw, J.S., J.R. Reimers, G.B. Bacska, A.T. Wong and N.S. Hush, Solitons in finite- and infinite-length negative-defect trans-polyacetylene and the corresponding Brooker (polymethinecyanine) cations. I. Geometry	167 (1992) 77

Craw, J.S., J.R. Reimers, G.B. Bacskey, A.T. Wong and N.S. Hush, Solitons in finite- and infinite-length negative-defect trans-polyacetylene and the corresponding Brooker (polymethinecyanine) cations. II. Charge density wave 167 (1992) 101

Cullin, D.W., see T.-Y.D. Lin 167 (1992) 203

Daudey, J.P., see A. Boutilib 167 (1992) 111

Delaire, J.A., see R. Loucif-Saïbi 167 (1992) 369

Denvir, D.J., see I.T.F. Gillan 167 (1992) 193

Di Bilio, A.J., see R.P. Bonomo 167 (1992) 385

Doisneau, G., see R. Loucif-Saïbi 167 (1992) 369

Domnin, I.N., see O. Schafer 167 (1992) 241

Duncan, I., see I.T.F. Gillan 167 (1992) 193

El Mouhtadi, M., see A. Boutilib 167 (1992) 111

Fillebeen-Khan, T., see R. Loucif-Saïbi 167 (1992) 369

Flament, J.P., N. Rougeau and M. Tadjeddine, Vibrational frequencies of simple sulfur oxides: ab initio SQM and MCSCF calculations; comparison 167 (1992) 53

Gillan, I.T.F., D.J. Denvir, H.F.J. Cormican, I. Duncan, T. Morrow and W.D. McGrath, 193 nm laser photodissociation of ClNO: initial vibrational energy distribution determined by LIF technique 167 (1992) 193

Granucci, G. and M. Persico, Electronic structure, vibrational spectrum and photochemistry of the Fe + H<sub>2</sub> system 167 (1992) 121

Gurman, V.S., see A.Kh. Vorobiev 167 (1992) 341

Hajigeorgiou, P.G., see J.A. Coxon 167 (1992) 327

Harigaya, K., Metal-insulator transition in doped conducting polymers. Disappearance of the electronic gap with persisting bond alternation in the system with site-type impurities 167 (1992) 315

Hush, N.S., see J.S. Craw 167 (1992) 77

Hush, N.S., see J.S. Craw 167 (1992) 101

Itoh, R., see F. Aiga 167 (1992) 277

Joyeux, M., The transition towards vibrational chaos in triatomic molecules. A numerical and analytical approach 167 (1992) 299

Kalinowski, J., W. Stapor, B. Petelenz and P. Petelenz, Electro-absorption spectrum of tetracene. High field measurements on polycrystalline samples 167 (1992) 185

Kopelman, R., see Z.-Y. Shi 167 (1992) 149

Ledoux, I., see R. Loucif-Saïbi 167 (1992) 369

Lee, S., see J. Sung 167 (1992) 17

Lin, T.-Y.D., X.-Q. Tan, T.M. Cerny, J.M. Williamson, D.W. Cullin and T.A. Miller, High-resolution fluorescence excitation spectra of jet-cooled benzyl and *p*-methylbenzyl radicals 167 (1992) 203

Loucif-Saïbi, R., J.A. Delaire, L. Bonazzola, G. Doisneau, G. Balavoine, T. Fillebeen-Khan, I. Ledoux and G. Puccetti, Molecular hyperpolarizabilities of new bimetallic ferrocenyl derivatives 167 (1992) 369

Marković, N., G. Nyman and S. Nordholm, Complex formation in  $X^+ + H_2$  collisions. Statistical estimation of ion-quadrupole capture rate constants 167 (1992) 157

McGrath, W.D., see I.T.F. Gillan 167 (1992) 193

Miller, T.A., see T.-Y.D. Lin 167 (1992) 203

Morrow, T., see I.T.F. Gillan 167 (1992) 193

Najbar, J., M. Boczar and A.M. Turek, Populations of the radical transients accompanying bimolecular electron transfer reactions in solutions 167 (1992) 37

Nordholm, S., see N. Marković 167 (1992) 157

Nyman, G., see N. Marković 167 (1992) 157

Palmer, M.H., see I.C. Walker 167 (1992) 61

Persico, M., see G. Granucci 167 (1992) 121

Petelenz, B., see J. Kalinowski 167 (1992) 185

Petelenz, P., see J. Kalinowski 167 (1992) 185

Petelenz, P., see M. Slawik 167 (1992) 377

Petrov, A.K., see A.B. Vakhtin 167 (1992) 1

Puccetti, G., see R. Loucif-Saïbi 167 (1992) 369

Rama Rao, K.V.S., see T. Bandyopadhyay 167 (1992) 131

Reimers, J.R., see J.S. Craw 167 (1992) 77

Reimers, J.R., see J.S. Craw 167 (1992) 101

Renge, I., On the determination of molecular polarizability changes upon electronic excitation from the solvent shifts of absorption band maxima 167 (1992) 173

Riggi, F., see R.P. Bonomo 167 (1992) 385

Røeggen, I. and P. Wind, A theoretical study of the  $(H_2)_2$  dimer. I. Bonding 167 (1992) 247

Røeggen, I., see P. Wind 167 (1992) 263

Rougeau, N., see J.P. Flament 167 (1992) 53

Sasagane, K., see F. Aiga 167 (1992) 277

Schafer, O., M. Allan, I.A. Boyarskaya and I.N. Domnin, Measurement of electron affinities of substituted cyclopropenes by electron transmission spectroscopy 167 (1992) 241

Sharafeddin, O.A., see D.H. Zhang 167 (1992) 137

Shi, Z.-Y. and R. Kopelman, Reaction order versus reaction probability for bimolecular steady state reactions:  $A + A \rightarrow A$  and  $A + A \rightarrow 0$  in one dimension 167 (1992) 149

Shin, K.J., see J. Sung 167 (1992) 17

Slawik, M. and P. Petelenz, Electro-absorption of charge transfer states: effect of sample texture 167 (1992) 377

Stampor, W., see J. Kalinowski 167 (1992) 185

Sung, J., K.J. Shin and S. Lee, Theory of diffusion-influenced fluorescence quenching. Effects of static quenching on the Stern-Volmer curve 167 (1992) 17

Tadjeddine, M., see J.P. Flament 167 (1992) 53

Tan, X.-Q., see T.-Y.D. Lin 167 (1992) 203

Thirunamachandran, T., see D.P. Craig 167 (1992) 229

Turek, A.M., see J. Najbar 167 (1992) 37

Vakhtin, A.B., A.V. Baklanov and A.K. Petrov, Absolute rate constants of  $R + NO(+M) \rightarrow RNO(+M)$  reactions. II. Measurements for  $R = C_2F_5$ ,  $i-C_3F_7$ ,  $n-C_4F_9$ , and  $t-C_4F_9$  at  $T = 295$  K 167 (1992) 1

Vorobiev, A.Kh. and V.S. Gurman, Investigation of hole mobility by photoorientation.  $X_2^-$  ions in glasses 167 (1992) 341

Walker, I.C., M.H. Palmer and C.C. Ballard, The electronic states of the azines. VI. 1,3,5-triazine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations 167 (1992) 61

Williams, J.H., Aspects of the vibrational spectroscopy of solid benzene and solid benzene:hexafluorobenzene 167 (1992) 215

Williamson, J.M., see T.-Y.D. Lin 167 (1992) 203

Wind, P., see I. Røeggen 167 (1992) 247

Wind, P. and I. Røeggen, A theoretical study of the  $(H_2)_2$  dimer. II. The potential energy surface 167 (1992) 263

Wong, A.T., see J.S. Craw 167 (1992) 77

Wong, A.T., see J.S. Craw 167 (1992) 101

Zhang, D.H., O.A. Sharafeddin and J.Z.H. Zhang, Product state distribution in time-dependent quantum wave packet calculation with an optical potential 167 (1992) 137

Zhang, J.Z.H., see D.H. Zhang 167 (1992) 137

## Subject Index to Volume 167

### Methods

#### Theoretical

##### *Quantized field theory*

An analysis of models for resonant transfer of excitation using quantum electrodynamics,  
D.P. Craig and T. Thirunamachandran

167 (1992) 229

##### *Statistical mechanics of stationary states*

Absolute rate constants of  $R + NO(+M) \rightarrow RNO(+M)$  reactions. II. Measurements for  
 $R = C_2F_5$ ,  $i-C_3F_7$ ,  $n-C_4F_9$ , and  $t-C_4F_9$  at  $T = 295$  K, A.B. Vakhtin, A.V. Baklanov and  
A.K. Petrov

167 (1992) 1

##### *Non-equilibrium thermodynamic and hydrodynamic theories*

Theory of diffusion-influenced fluorescence quenching. Effects of static quenching on the  
Stern-Volmer curve, J. Sung, K.J. Shin and S. Lee

167 (1992) 17

Populations of the radical transients accompanying bimolecular electron transfer reactions  
in solutions, J. Najbar, M. Boczar and A.M. Turek

167 (1992) 37

##### *Ab initio schemes for stationary properties*

Vibrational frequencies of simple sulfur oxides: ab initio SQM and MCSCF calculations;  
comparison, J.P. Flament, N. Rougeau and M. Tadjeddine

167 (1992) 53

The electronic states of the azines. VI. 1,3,5-triazine, studied by VUV absorption, near-  
threshold electron energy-loss spectroscopy and ab initio multi-reference configuration  
interaction calculations, I.C. Walker, M.H. Palmer and C.C. Ballard

167 (1992) 61

Solitons in finite- and infinite-length negative-defect trans-polyacetylene and the corre-  
sponding Brooker (polymethinecyanine) cations. II. Charge density wave, J.S. Craw,  
J.R. Reimers, G.B. Bacska, A.T. Wong and N.S. Hush

167 (1992) 101

Theoretical study of the lowest electronic states of  $CaH$  and  $CaH^+$  molecules, A. Boutalib,  
J.P. Daudey and M. El Mouhtadi

167 (1992) 111

Electronic structure, vibrational spectrum and photochemistry of the  $Fe + H_2$  system,  
G. Granucci and M. Persico

167 (1992) 121

Measurement of electron affinities of substituted cyclopropenes by electron transmission  
spectroscopy, O. Schafer, M. Allan, I.A. Boyarskaya and I.N. Dominin

167 (1992) 241

A theoretical study of the  $(H_2)_2$  dimer. I. Bonding, I. Røeggen and P. Wind

167 (1992) 247

A theoretical study of the  $(H_2)_2$  dimer. II. The potential energy surface, P. Wind and  
I. Røeggen

167 (1992) 263

The quadratic response function in the TDHF approximation and its application to frequency-dependent hyperpolarizabilities of the FH molecule, F. Aiga, K. Sasagane and R. Itoh	167 (1992) 277
Ab initio study of the oxides of rhenium and their anions, R.C. Boehm and A. Banerjee	167 (1992) 291
<i>Computational and simulation methods</i>	
Solitons in finite- and infinite-length negative-defect trans-polyacetylene and the corresponding Brooker (polymethinecyanine) cations. I. Geometry, J.S. Craw, J.R. Reimers, G.B. Bacska, A.T. Wong and N.S. Hush	167 (1992) 77
Excitation transfer by long-range and short-range interactions in liquid solution: the temporal behavior, T. Bandyopadhyay and K.V.S. Rama Rao	167 (1992) 131
Reaction order versus reaction probability for bimolecular steady state reactions: $A + A \rightarrow A$ and $A + A \rightarrow 0$ in one dimension, Z.-Y. Shi and R. Kopelman	167 (1992) 149
The transition towards vibrational chaos in triatomic molecules. A numerical and analytical approach, M. Joyeux	167 (1992) 299
Metal-insulator transition in doped conducting polymers. Disappearance of the electronic gap with persisting bond alternation in the system with site-type impurities, K. Harigaya	167 (1992) 315
On the direct determination of analytical diatomic potential energy functions from spectroscopic data: the $X^1\Sigma^+$ electronic states of NaF, LiI, CS, and SiS, J.A. Coxon and P.G. Hajigeorgiou	167 (1992) 327
<i>Molecular dynamics and scattering theory</i>	
Product state distribution in time-dependent quantum wave packet calculation with an optical potential, D.H. Zhang, O.A. Sharafeddin and J.Z.H. Zhang	167 (1992) 137
Complex formation in $X^+ + H_2$ collisions. Statistical estimation of ion-quadrupole capture rate constants, N. Marković, G. Nyman and S. Nordholm	167 (1992) 157
The transition towards vibrational chaos in triatomic molecules. A numerical and analytical approach, M. Joyeux	167 (1992) 299
Investigation of hole mobility by photoorientation. $X_2^-$ ions in glasses, A.Kh. Vorobiev and V.S. Gurman	167 (1992) 341
<i>Experimental</i>	
<i>Magnetic resonances</i>	
Investigation of hole mobility by photoorientation. $X_2^-$ ions in glasses, A.Kh. Vorobiev and V.S. Gurman	167 (1992) 341
<i>Infrared spectroscopy</i>	
Vibrational frequencies of simple sulfur oxides: ab initio SQM and MCSCF calculations; comparison, J.P. Flament, N. Rougeau and M. Tadjeeddine	167 (1992) 53
<i>Visible and UV spectroscopy</i>	
On the determination of molecular polarizability changes upon electronic excitation from the solvent shifts of absorption band maxima, I. Renge	167 (1992) 173
Electro-absorption spectrum of tetracene. High field measurements on polycrystalline samples, J. Kalinowski, W. Stampor, B. Petelenz and P. Petelenz	167 (1992) 185
Investigation of hole mobility by photoorientation. $X_2^-$ ions in glasses, A.Kh. Vorobiev and V.S. Gurman	167 (1992) 341

Absolute oscillator strengths for photoabsorption (6–360 eV) and ionic photodissociation (10–80 eV) of methanol, G.R. Burton, W.F. Chan, G. Cooper and C.E. Brion 167 (1992) 349

Molecular hyperpolarizabilities of new bimetallic ferrocenyl derivatives, R. Loucif-Saïbi, J.A. Delaire, L. Bonazzola, G. Doisneau, G. Balavoine, T. Fillebeen-Khan, I. Ledoux and G. Puccetti 167 (1992) 369

Electro-absorption of charge transfer states: effect of sample texture, M. Slawik and P. Petelenz 167 (1992) 377

*Fluorescence spectroscopy*

193 nm laser photodissociation of CINO: initial vibrational energy distribution determined by LIF technique, I.T.F. Gillan, D.J. Denvir, H.F.J. Cormican, I. Duncan, T. Morrow and W.D. McGrath 167 (1992) 193

*X-ray spectroscopy*

Absolute oscillator strengths for photoabsorption (6–360 eV) and ionic photodissociation (10–80 eV) of methanol, G.R. Burton, W.F. Chan, G. Cooper and C.E. Brion 167 (1992) 349

*Electron impact spectroscopy*

The electronic states of the azines. VI. 1,3,5-triazine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker, M.H. Palmer and C.C. Ballard 167 (1992) 61

Measurement of electron affinities of substituted cyclopropenes by electron transmission spectroscopy, O. Schafer, M. Allan, I.A. Boyarskaya and I.N. Domnin 167 (1992) 241

*Laser methods*

Absolute rate constants of R+NO(+M)→RNO(+M) reactions. II. Measurements for R=C<sub>2</sub>F<sub>5</sub>, *i*-C<sub>3</sub>F<sub>7</sub>, *n*-C<sub>4</sub>F<sub>9</sub>, and *t*-C<sub>4</sub>F<sub>9</sub> at T=295 K, A.B. Vakhtin, A.V. Baklanov and A.K. Petrov 167 (1992) 1

193 nm laser photodissociation of CINO: initial vibrational energy distribution determined by LIF technique, I.T.F. Gillan, D.J. Denvir, H.F.J. Cormican, I. Duncan, T. Morrow and W.D. McGrath 167 (1992) 193

High-resolution fluorescence excitation spectra of jet-cooled benzyl and *p*-methylbenzyl radicals, T.-Y.D. Lin, X.-Q. Tan, T.M. Cerny, J.M. Williamson, D.W. Cullin and T.A. Miller 167 (1992) 203

*Non-linear optical spectroscopy*

Molecular hyperpolarizabilities of new bimetallic ferrocenyl derivatives, R. Loucif-Saïbi, J.A. Delaire, L. Bonazzola, G. Doisneau, G. Balavoine, T. Fillebeen-Khan, I. Ledoux and G. Puccetti 167 (1992) 369

*Synchrotron spectroscopies*

The electronic states of the azines. VI. 1,3,5-triazine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker, M.H. Palmer and C.C. Ballard 167 (1992) 61

*Coherent optical spectroscopy*

Investigation of hole mobility by photoorientation. X<sub>2</sub><sup>-</sup> ions in glasses, A.Kh. Vorobiev and V.S. Gurman 167 (1992) 341

*Time-resolved experiments*

Absolute rate constants of  $R + NO(+M) \rightarrow RNO(+M)$  reactions. II. Measurements for  $R = C_2F_5$ ,  $i-C_3F_7$ ,  $n-C_4F_9$ , and  $t-C_4F_9$  at  $T = 295$  K, A.B. Vakhtin, A.V. Baklanov and A.K. Petrov

167 (1992) 1

*Neutron scattering*

Aspects of the vibrational spectroscopy of solid benzene and solid benzene:hexafluorobenzene, J.H. Williams

167 (1992) 215

**Objects****Bulk systems***Gases*

Vibrational frequencies of simple sulfur oxides: ab initio SQM and MCSCF calculations; comparison, J.P. Flament, N. Rougeau and M. Tadjeeddine

167 (1992) 53

A theoretical study of the  $(H_2)_2$  dimer. I. Bonding, I. Røeggen and P. Wind

167 (1992) 247

A theoretical study of the  $(H_2)_2$  dimer. II. The potential energy surface, P. Wind and I. Røeggen

167 (1992) 263

*Liquids mixtures and solutions*

Theory of diffusion-influenced fluorescence quenching. Effects of static quenching on the Stern-Volmer curve, J. Sung, K.J. Shin and S. Lee

167 (1992) 17

Excitation transfer by long-range and short-range interactions in liquid solution: the temporal behavior, T. Bandyopadhyay and K.V.S. Rama Rao

167 (1992) 131

On the determination of molecular polarizability changes upon electronic excitation from the solvent shifts of absorption band maxima, I. Renge

167 (1992) 173

*Crystals**-neat*

Electro-absorption spectrum of tetracene. High field measurements on polycrystalline samples, J. Kalinowski, W. Stapor, B. Petelenz and P. Petelenz

167 (1992) 185

Electro-absorption of charge transfer states: effect of sample texture, M. Slawik and P. Petelenz

167 (1992) 377

*Glasses*

Investigation of hole mobility by photoorientation.  $X_2^-$  ions in glasses, A.Kh. Vorobiev and V.S. Gurman

167 (1992) 341

*Polymers*

Solitons in finite- and infinite-length negative-defect trans-polyacetylene and the corresponding Brooker (polymethinecyanine) cations. I. Geometry, J.S. Craw, J.R. Reimers, G.B. Bacska, A.T. Wong and N.S. Hush

167 (1992) 77

Solitons in finite- and infinite-length negative-defect trans-polyacetylene and the corresponding Brooker (polymethinecyanine) cations. II. Charge density wave, J.S. Craw, J.R. Reimers, G.B. Bacskay, A.T. Wong and N.S. Hush 167 (1992) 101

Metal-insulator transition in doped conducting polymers. Disappearance of the electronic gap with persisting bond alternation in the system with site-type impurities, K. Harigaya 167 (1992) 315

*Thin films*

Electro-absorption of charge transfer states: effect of sample texture, M. Slawik and P. Petelenz 167 (1992) 377

*Surfaces*

Product state distribution in time-dependent quantum wave packet calculation with an optical potential, D.H. Zhang, O.A. Sharafeddin and J.Z.H. Zhang 167 (1992) 137

*Low-dimensional materials*

Reaction order versus reaction probability for bimolecular steady state reactions:  $A + A \rightarrow A$  and  $A + A \rightarrow 0$  in one dimension, Z.-Y. Shi and R. Kopelman 167 (1992) 149

Metal-insulator transition in doped conducting polymers. Disappearance of the electronic gap with persisting bond alternation in the system with site-type impurities, K. Harigaya 167 (1992) 315

*Microscopic systems*

*Molecules (neutral and ionic)*

Vibrational frequencies of simple sulfur oxides: ab initio SQM and MCSCF calculations; comparison, J.P. Flament, N. Rougeau and M. Tadjeddine 167 (1992) 53

The quadratic response function in the TDHF approximation and its application to frequency-dependent hyperpolarizabilities of the FH molecule, F. Aiga, K. Sasagane and R. Itoh 167 (1992) 277

*-diatomic*

Theoretical study of the lowest electronic states of CaH and  $CaH^+$  molecules, A. Boutalib, J.P. Daudey and M. El Mouhtadi 167 (1992) 111

Product state distribution in time-dependent quantum wave packet calculation with an optical potential, D.H. Zhang, O.A. Sharafeddin and J.Z.H. Zhang 167 (1992) 137

Complex formation in  $X^+ + H_2$  collisions. Statistical estimation of ion-quadrupole capture rate constants, N. Marković, G. Nyman and S. Nordholm 167 (1992) 157

On the direct determination of analytical diatomic potential energy functions from spectroscopic data: the  $X^1\Sigma^+$  electronic states of NaF, LiI, CS, and SiS, J.A. Coxon and P.G. Hajigeorgiou 167 (1992) 327

*-small polyatomics*

The electronic states of the azines. VI. 1,3,5-triazine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker, M.H. Palmer and C.C. Ballard 167 (1992) 61

Electronic structure, vibrational spectrum and photochemistry of the  $Fe + H_2$  system, G. Granucci and M. Persico 167 (1992) 121

193 nm laser photodissociation of ClNO: initial vibrational energy distribution determined by LIF technique, I.T.F. Gillan, D.J. Denvir, H.F.J. Cormican, I. Duncan, T. Morrow and W.D. McGrath	167 (1992) 193
The transition towards vibrational chaos in triatomic molecules. A numerical and analytical approach, M. Joyeux	167 (1992) 299
Absolute oscillator strengths for photoabsorption (6–360 eV) and ionic photofragmentation (10–80 eV) of methanol, G.R. Burton, W.F. Chan, G. Cooper and C.E. Brion	167 (1992) 349
<i>-aromatics</i>	
On the determination of molecular polarizability changes upon electronic excitation from the solvent shifts of absorption band maxima, I. Renge	167 (1992) 173
Electro-absorption spectrum of tetracene. High field measurements on polycrystalline samples, J. Kalinowski, W. Stapor, B. Petelenz and P. Petelenz	167 (1992) 185
<i>-other large</i>	
Measurement of electron affinities of substituted cyclopropenes by electron transmission spectroscopy, O. Schafer, M. Allan, I.A. Boyarskaya and I.N. Dominin	167 (1992) 241
<i>Molecular aggregates</i>	
<i>-dimers</i>	
A theoretical study of the $(H_2)_2$ dimer. I. Bonding, I. Røeggen and P. Wind	167 (1992) 247
A theoretical study of the $(H_2)_2$ dimer. II. The potential energy surface, P. Wind and I. Røeggen	167 (1992) 263
<i>-van der Waals molecules</i>	
A theoretical study of the $(H_2)_2$ dimer. I. Bonding, I. Røeggen and P. Wind	167 (1992) 247
A theoretical study of the $(H_2)_2$ dimer. II. The potential energy surface, P. Wind and I. Røeggen	167 (1992) 263
<i>-complexes</i>	
Molecular hyperpolarizabilities of new bimetallic ferrocenyl derivatives, R. Loucif-Saïbi, J.A. Delaire, L. Bonazzola, G. Doisneau, G. Balavoine, T. Fillebeen-Khan, I. Ledoux and G. Puccetti	167 (1992) 369
<i>Free radicals (including hydronium and muonium)</i>	
Absolute rate constants of $R + NO(+M) \rightarrow RNO(+M)$ reactions. II. Measurements for $R = C_2F_5$ , $i-C_3F_7$ , $n-C_4F_9$ , and $t-C_4F_9$ at $T = 295$ K, A.B. Vakhtin, A.V. Baklanov and A.K. Petrov	167 (1992) 1
Populations of the radical transients accompanying bimolecular electron transfer reactions in solutions, J. Najbar, M. Boczar and A.M. Turek	167 (1992) 37

*Quasiparticles (including excitons)*

Electro-absorption of charge transfer states: effect of sample texture, M. Slawik and P. Petelenz 167 (1992) 377

*Ions and charge carriers*

Solitons in finite- and infinite-length negative-defect trans-polyacetylene and the corresponding Brooker (polymethinecyanine) cations. I. Geometry, J.S. Craw, J.R. Reimers, G.B. Bacska, A.T. Wong and N.S. Hush 167 (1992) 77

Solitons in finite- and infinite-length negative-defect trans-polyacetylene and the corresponding Brooker (polymethinecyanine) cations. II. Charge density wave, J.S. Craw, J.R. Reimers, G.B. Bacska, A.T. Wong and N.S. Hush 167 (1992) 101

Measurement of electron affinities of substituted cyclopropenes by electron transmission spectroscopy, O. Schafer, M. Allan, I.A. Boyarskaya and I.N. Dominin 167 (1992) 241

Ab initio study of the oxides of rhenium and their anions, R.C. Boehm and A. Banerjee 167 (1992) 291

**Phenomena***Molecular structure*

Solitons in finite- and infinite-length negative-defect trans-polyacetylene and the corresponding Brooker (polymethinecyanine) cations. I. Geometry, J.S. Craw, J.R. Reimers, G.B. Bacska, A.T. Wong and N.S. Hush 167 (1992) 77

Solitons in finite- and infinite-length negative-defect trans-polyacetylene and the corresponding Brooker (polymethinecyanine) cations. II. Charge density wave, J.S. Craw, J.R. Reimers, G.B. Bacska, A.T. Wong and N.S. Hush 167 (1992) 101

High-resolution fluorescence excitation spectra of jet-cooled benzyl and *p*-methylbenzyl radicals, T.-Y.D. Lin, X.-Q. Tan, T.M. Cerny, J.M. Williamson, D.W. Cullin and T.A. Miller 167 (1992) 203

*Vibrations and rotations of molecules*

Vibrational frequencies of simple sulfur oxides: ab initio SQM and MCSCF calculations; comparison, J.P. Flament, N. Rougeau and M. Tadjeddine 167 (1992) 53

Electronic structure, vibrational spectrum and photochemistry of the Fe + H<sub>2</sub> system, G. Granucci and M. Persico 167 (1992) 121

Aspects of the vibrational spectroscopy of solid benzene and solid benzene:hexafluorobenzene, J.H. Williams 167 (1992) 215

The transition towards vibrational chaos in triatomic molecules. A numerical and analytical approach, M. Joyeux 167 (1992) 299

On the direct determination of analytical diatomic potential energy functions from spectroscopic data: the X<sup>1</sup>Σ<sup>+</sup> electronic states of NaF, LiI, CS, and SiS, J.A. Coxon and P.G. Hajigeorgiou 167 (1992) 327

*Electronic structure and states*

The electronic states of the azines. VI. 1,3,5-triazine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker, M.H. Palmer and C.C. Ballard 167 (1992) 61

Theoretical study of the lowest electronic states of CaH and CaH<sup>+</sup> molecules, A. Boutalib, J.P. Daudey and M. El Mouhtadi 167 (1992) 111

Electronic structure, vibrational spectrum and photochemistry of the Fe+H<sub>2</sub> system, G. Granucci and M. Persico 167 (1992) 121

Electro-absorption spectrum of tetracene. High field measurements on polycrystalline samples, J. Kalinowski, W. Stampor, B. Petelenz and P. Petelenz 167 (1992) 185

Measurement of electron affinities of substituted cyclopropenes by electron transmission spectroscopy, O. Schafer, M. Allan, I.A. Boyarskaya and I.N. Dominin 167 (1992) 241

Ab initio study of the oxides of rhenium and their anions, R.C. Boehm and A. Banerjee 167 (1992) 291

Metal-insulator transition in doped conducting polymers. Disappearance of the electronic gap with persisting bond alternation in the system with site-type impurities, K. Harigaya 167 (1992) 315

*Electric and magnetic properties*

The quadratic response function in the TDHF approximation and its application to frequency-dependent hyperpolarizabilities of the FH molecule, F. Aiga, K. Sasagane and R. Itoh 167 (1992) 277

*Molecular interactions*

Product state distribution in time-dependent quantum wave packet calculation with an optical potential, D.H. Zhang, O.A. Sharafeddin and J.Z.H. Zhang 167 (1992) 137

Complex formation in X<sup>+</sup> + H<sub>2</sub> collisions. Statistical estimation of ion-quadrupole capture rate constants, N. Marković, G. Nyman and S. Nordholm 167 (1992) 157

Aspects of the vibrational spectroscopy of solid benzene and solid benzene:hexafluorobenzene, J.H. Williams 167 (1992) 215

An analysis of models for resonant transfer of excitation using quantum electrodynamics, D.P. Craig and T. Thirunamachandran 167 (1992) 229

A theoretical study of the (H<sub>2</sub>)<sub>2</sub> dimer. I. Bonding, I. Røeggen and P. Wind 167 (1992) 247

A theoretical study of the (H<sub>2</sub>)<sub>2</sub> dimer. II. The potential energy surface, P. Wind and I. Røeggen 167 (1992) 263

*Spectral bandshapes and intensities*

Absolute oscillator strengths for photoabsorption (6–360 eV) and ionic photofragmentation (10–80 eV) of methanol, G.R. Burton, W.F. Chan, G. Cooper and C.E. Brion 167 (1992) 349

Electro-absorption of charge transfer states: effect of sample texture, M. Slawik and P. Petelenz 167 (1992) 377

*Coupling of electronic and nuclear motion*

On the direct determination of analytical diatomic potential energy functions from spectroscopic data: the X<sup>1</sup>Σ<sup>+</sup> electronic states of NaF, LiI, CS, and SiS, J.A. Coxon and P.G. Hajigeorgiou 167 (1992) 327

*Energy transfer processes*

Theory of diffusion-influenced fluorescence quenching. Effects of static quenching on the Stern–Volmer curve, J. Sung, K.J. Shin and S. Lee 167 (1992) 17

Excitation transfer by long-range and short-range interactions in liquid solution: the temporal behavior, T. Bandyopadhyay and K.V.S. Rama Rao 167 (1992) 131

An analysis of models for resonant transfer of excitation using quantum electrodynamics, D.P. Craig and T. Thirunamachandran 167 (1992) 229

*Molecular photophysical processes*

On the determination of molecular polarizability changes upon electronic excitation from the solvent shifts of absorption band maxima, I. Renge 167 (1992) 173

Electro-absorption spectrum of tetracene. High field measurements on polycrystalline samples, J. Kalinowski, W. Stämpfli, B. Petelenz and P. Petelenz 167 (1992) 185

193 nm laser photodissociation of ClNO: initial vibrational energy distribution determined by LIF technique, I.T.F. Gillan, D.J. Denvir, H.F.J. Cormican, I. Duncan, T. Morrow and W.D. McGrath 167 (1992) 193

Absolute oscillator strengths for photoabsorption (6–360 eV) and ionic photofragmentation (10–80 eV) of methanol, G.R. Burton, W.F. Chan, G. Cooper and C.E. Brion 167 (1992) 349

*Intramolecular dynamics**–vibrational energy redistribution (including vibrational dissociation)*

193 nm laser photodissociation of ClNO: initial vibrational energy distribution determined by LIF technique, I.T.F. Gillan, D.J. Denvir, H.F.J. Cormican, I. Duncan, T. Morrow and W.D. McGrath 167 (1992) 193

*Luminescence spectra, yields and lifetimes*

Theory of diffusion-influenced fluorescence quenching. Effects of static quenching on the Stern–Volmer curve, J. Sung, K.J. Shin and S. Lee 167 (1992) 17

*Non-linear responses (including optical)*

The quadratic response function in the TDHF approximation and its application to frequency-dependent hyperpolarizabilities of the FH molecule, F. Aiga, K. Sasagane and R. Itoh 167 (1992) 277

Molecular hyperpolarizabilities of new bimetallic ferrocenyl derivatives, R. Loucif-Saïbi, J.A. Delaire, L. Bonazzola, G. Doisneau, G. Balavoine, T. Fillebeen-Khan, I. Ledoux and G. Puccetti 167 (1992) 369

*Reactions (including dissociation)*

Product state distribution in time-dependent quantum wave packet calculation with an optical potential, D.H. Zhang, O.A. Sharafeddin and J.Z.H. Zhang 167 (1992) 137

*–gas phase*

Absolute rate constants of R + NO(+M) → RNO(+M) reactions. II. Measurements for R = C<sub>2</sub>F<sub>5</sub>, i-C<sub>3</sub>F<sub>7</sub>, n-C<sub>4</sub>F<sub>9</sub>, and t-C<sub>4</sub>F<sub>9</sub> at T = 295 K, A.B. Vakhtin, A.V. Baklanov and A.K. Petrov 167 (1992) 1

Complex formation in X<sup>+</sup> + H<sub>2</sub> collisions. Statistical estimation of ion–quadrupole capture rate constants, N. Marković, G. Nyman and S. Nordholm 167 (1992) 157

*–condensed phase*

Theory of diffusion-influenced fluorescence quenching. Effects of static quenching on the Stern–Volmer curve, J. Sung, K.J. Shin and S. Lee 167 (1992) 17

Reaction order versus reaction probability for bimolecular steady state reactions: $A + A \rightarrow A$ and $A + A \rightarrow 0$ in one dimension, Z.-Y. Shi and R. Kopelman	167 (1992) 149
<i>-photochemical</i>	
Populations of the radical transients accompanying bimolecular electron transfer reactions in solutions, J. Najbar, M. Boczar and A.M. Turek	167 (1992) 37
Electronic structure, vibrational spectrum and photochemistry of the $Fe + H_2$ system, G. Granucci and M. Persico	167 (1992) 121
<i>Electron transfer</i>	
Populations of the radical transients accompanying bimolecular electron transfer reactions in solutions, J. Najbar, M. Boczar and A.M. Turek	167 (1992) 37
Solitons in finite- and infinite-length negative-defect trans-polyacetylene and the corresponding Brooker (polymethinecyanine) cations. I. Geometry, J.S. Craw, J.R. Reimers, G.B. Bacska, A.T. Wong and N.S. Hush	167 (1992) 77
Solitons in finite- and infinite-length negative-defect trans-polyacetylene and the corresponding Brooker (polymethinecyanine) cations. II. Charge density wave, J.S. Craw, J.R. Reimers, G.B. Bacska, A.T. Wong and N.S. Hush	167 (1992) 101
<i>Ionization (including Rydberg states)</i>	
Ab initio study of the oxides of rhenium and their anions, R.C. Boehm and A. Banerjee	167 (1992) 291
<i>Molecular motion (including diffusive)</i>	
Populations of the radical transients accompanying bimolecular electron transfer reactions in solutions, J. Najbar, M. Boczar and A.M. Turek	167 (1992) 37
<i>Isotopic effects</i>	
On the direct determination of analytical diatomic potential energy functions from spectroscopic data: the $X^1\Sigma^+$ electronic states of $NaF$ , $LiI$ , $CS$ , and $SiS$ , J.A. Coxon and P.G. Hajigeorgiou	167 (1992) 327
<i>Collective motion and excitations</i>	
Aspects of the vibrational spectroscopy of solid benzene and solid benzene:hexafluorobenzene, J.H. Williams	167 (1992) 215
<i>Surface effects and catalysis</i>	
Ab initio study of the oxides of rhenium and their anions, R.C. Boehm and A. Banerjee	167 (1992) 291
<i>Structure of solids and liquids</i>	
Metal-insulator transition in doped conducting polymers. Disappearance of the electronic gap with persisting bond alternation in the system with site-type impurities, K. Harigaya	167 (1992) 315